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SOLIDS
AND LIQUIDS

Dynamics of Liquid Lithium Atoms. Pseudopotential and EAM-Type Potentials

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Abstract—It is generally accepted that the complicated character of the interparticle interaction in liquid metals is reproduced most correctly by many-particle potentials of the EAM-type (embedded atom model) interparticle interaction. It is shown that in the case of liquid lithium near the melting temperature ($T_m = 453.65$ K), the spherical pseudopotential provides a better agreement with experimental data on elastic and inelastic X-ray scattering as compared to the known EAM potentials. The calculations of the dynamic structural factor and spectral densities of the longitudinal and transverse atomic currents lead to the conclusion that although the pseudopotential and EAM potentials generate a certain qualitative correspondence in the features of collective dynamics, the interparticle interaction of the spherical type reproduces correctly the general form of the dynamic structure factor in a certain wavenumber range, as well as the dispersion relation for collective excitations.

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1. INTRODUCTION

Among other alkali metals, lithium has the simplest electronic structure $1s^2 2s^1$ (two inner *s*-electrons and one valence electron). According to the number of nucleon and electrons, lithium can be considered as the simplest metal existing in nature [1, 2]. Nevertheless, many properties of lithium melt are quite nontrivial, due to the specific ion–ion interaction [3], even as compared to other liquid alkali metals. For example, the potentials constructed on the basis of the local pseudopotential (e.g., Ashcroft potential [4]) for lithium cannot be used for reproducing the structure or dynamics, while such potentials for other alkali metals are in good agreement with experiments in a wide temperature range. This is partly due to the fact that the number of conduction electrons in lithium constitutes about 33% of their total number, while these fractions for sodium and cesium are 9% and 1.8%, respectively. Further, lithium practically does not mix with other alkali elements, while other alkali metals can form homogeneous mixtures (for example, we can mention sodium–potassium, cesium–rubidium, or cesium–potassium alloys) [5]. Lithium exhibits a higher chemical stability as compared to other alkali metals and forms compounds with many nonalkali metals, which are characterized by a high melting point and hardness [6]. Owing to its high specific heat and thermal conductivity, as well as low viscosity and density, liquid lithium can be effectively used as a coolant in uranium reactors in atomic power production [7].

For reproducing the interparticle interaction in liquid lithium, various model potentials were proposed, including local [8, 9] and nonlocal [10, 11] potentials, effective [12] spherical potentials (see review [13]), as well as many-particle EAM-type potentials (embedded atom method) [14, 15] and their modifications (modified embedded atom model, MEAM) [16]. Remarkably, in accordance with a large number of methods for developing interparticle interaction potentials, the potential parameters are selected from the very outset for reproducing correctly separate regions of the phase diagram as well as structural properties. Obviously, the "correct" structure does not imply the generation of the correct dynamics and transport properties by a potential. The main goal of this study is to analyze the accuracy of the description of the structure and the microscopic dynamics of liquid lithium in the vicinity of the melting temperature using different potentials of interparticle interaction, namely, the effective spherical pseudopotential [12], the embedded atom potential (many-particle EAM potential) [15], and modified embedded atom model potential (MEAM potential) [16].

2. STRUCTURE AND COLLECTIVE DYNAMICS OF LITHIUM ATOMS

We consider an equilibrium lithium melt at temperature $T = 475$ K with concentration $\rho = 0.0445$ Å^{-3}. Such a (ρ, T)-state is close to the melting curve, and its structure and collective atomic dynamics have investi-